

## **Exhibit One**

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# Data handling causes image problem for top lab

Two papers — one published more than a decade ago and the other a preprint from last year — have raised doubts among experts about the work of a world-renowned microscopy laboratory.

In a Corrigendum in this week's issue of *Nature* (see page 235), three authors from an atomic-imaging group at Oak Ridge National Laboratory in Tennessee admit to treating critical data inconsistently in a paper from 1993 (ref. 1). Two of the three authors are also co-authors on an August 2005 paper, on the arxiv.org preprint server<sup>2</sup>, in which some data were reproduced from one of the group's earlier papers<sup>3</sup> without citation and another figure included duplicated data points on two sides of a plot. The authors posted a revised version, with added citations and a replacement figure, on 15 May 2006 (ref. 4).

An investigation over the summer by an independent panel, formed at the behest of the Oak Ridge lab, found "no evidence of research misconduct or fraud in either paper", according to James Roberto, the lab's deputy director for science and technology.

But within the community, doubts linger. "It's obvious that some games are being played," comments John Silcox of Cornell University in Ithaca, New York, who was a reviewer of the 1993 *Nature* article. "I don't trust their work."

Few researchers were willing to go on the record, but several told *Nature* privately that they also were concerned about the papers.

The group is led by Stephen Pennycook, a physicist who has been at Oak Ridge since 1982. His group helped pioneer the scanning transmission electron microscope (STEM), which uses a narrow beam of electrons to simultaneously take spectra of and image materials. The microscopes cost millions of dollars and the field is intensely competitive. Pennycook's group is at the forefront, says John Spence, a physicist at Arizona State University in Tempe: "They have the



Questions have arisen over data from a team at Oak Ridge National Laboratory.

best machine, the most money, and very good people."

In the *Nature* paper, the collaboration reported taking spectra and images of a boundary between a thin wafer of cobalt silicide and one of silicon. At the time, imaging such an interface was difficult. The team proved it was possible by showing clear spectra of both the cobalt silicide and silicon.

But in the Corrigendum, the authors admit that the cobalt silicide spectra were reproduced from an earlier conference paper by the same group<sup>5</sup>. The admission contradicts the authors' response to a 1993 referee report (obtained independently and verified by *Nature*'s news team) in which they deny that the spectra came from the proceedings. Pennycook says that the original statements were made because the group was confused about the referee's criticisms.

The duplication of some but not all spectra meant that different methods were used to process the background noise on either side of the boundary. Some researchers are unfazed by the error: "Clearly it's a minor mistake, but fundamentally it has no influence on the results," says Christian Colliex, head of the STEM group at the University of Paris South, who collaborates with Pennycook but had no role in the 1993 paper. But others believe the

mistake should invalidate the result. "I don't understand why they haven't retracted this paper," says Silcox. *Nature*'s view is given on page 123.

The more recent arxiv.org paper is also a study of the boundary between two materials: one ferromagnetic and one superconducting. In the first version of the paper<sup>2</sup>, several graphs and one image appear identical to those in an earlier paper by the group<sup>3</sup>. In addition, a plot in the paper contains identical but mirrored data on its right- and left-hand sides. "It looks fishy," says David Muller, a physicist at Cornell, who obtained his PhD under Silcox.

The paper was first posted at arxiv.org on 23 August 2005. Others in the field became aware of the irregularities in the spring of 2006, when a version was submitted to *Nature Physics*, according to sources outside *Nature* familiar with its history. Within days of being notified of the issues, the authors posted a revised version<sup>4</sup>, which added references for all but one image. It also contained a version of the data plot that had been cropped in a way that eliminates the duplicated data points.

In a phone interview, Pennycook and lead author Maria Valera admitted that the data were duplicated on either side of the plot: "I think it was an effort to make it look more attractive to *Nature*

editors, frankly," Pennycook says. "It was the wrong thing to do," adds Valera. She says she was the first to use the mirrored data plot, at an American Physical Society conference, but she does not recall who originally put the plot together. Valera also admits that she did not appropriately cite the earlier paper<sup>3</sup> from which several figures were reproduced.

"Obviously mistakes have happened," says Pennycook. "Mistakes always happen in science." He says that he believes the criticisms spring primarily from his rivals at Cornell, and adds that he stands by his work: "A lot of people think we are the number one group in the world," he says. "We have no reason to say anything that's not absolutely right."

The investigating panel of three scientists found "errors in judgement", but no evidence of falsification or fabrication, says panel member Paul Peercy, dean of engineering at the University of Wisconsin at Madison. He says that they concluded that the graph with mirrored data was improperly presented, but that it did not change the paper's core result. "In today's world of PowerPoint," he says, "there is a tendency to present data in whatever the author may think is the best form."

But some in the field continue to have doubts. "There is a pattern of sloppiness here," says Spence. "This is very troubling."

Geoff Brumfiel

1. Browning, N. D., Chisholm, M. F. & Pennycook, S. J. *Nature* **366**, 143–146 (1993)
2. Varela, M. et al. arxiv.org/pdf/cond-mat/0508564v1 (2005)
3. Varela, M. et al. *Solid State Electron.* **47**, 2245–2248 (2003)
4. Varela, M. et al. arxiv.org/pdf/cond-mat/0508564 (2006).
5. Browning, N. D. et al. in *Sist Ann. Proc. Microsc. Soc. Am.* 576–577 (San Francisco Press, California, 1993).

**Editor's note:** In keeping with *Nature*'s practice of confidentiality, *Nature*'s news team was provided with no access to any material pertaining to either of the papers other than the text of the Corrigendum itself.

# Another one bites the dust

The hazards of seeking to implement reforms at universities with outstanding reputations have been demonstrated once again, this time in Switzerland.

Switzerland's flagship university, the Swiss Federal Institute of Technology (ETH) in Zurich, is arguably the strongest in mainland Europe. The government already provides one of the highest per-capita expenditures on research in the world, and is set to increase funding by a further 30% over the next five years.

But if nothing seems to be broken, does anything need fixing? Ernst Hafen, the molecular biologist who became president of the ETH last December, thought it did. In his view, major reforms were required in order to safeguard the university's pre-eminence. Unlike most Swiss universities, where deans share decision-making, the ETH president's position is a powerful one and, in theory, Hafen should have been able to have his way.

But the ETH faculty put paid to that, pulling rank after a short but bitter public dispute and securing Hafen's resignation just eleven months in (see page 130). The hostility of the ETH faculty to the man who wanted to restructure it echoes that attracted by Larry Summers at Harvard University two years ago (see *Nature* 433, 190–192; 2005), which culminated in a row over his unfortunate comments on the aptitude of women and his subsequent resignation.

Hafen had been impressed by a previous, successful reorganization five years ago at the other federally funded university in Switzerland, the EFP Lausanne — the remaining universities in Switzerland are funded by their local cantons — and wanted to introduce a more corporate management model at the ETH.

The ETH currently has little hierarchy below the president, and what there is mostly concentrates in the *Schulleitung*, comprising the president, two vice-presidents (responsible for research and infrastructure) and the faculty-elected rector (responsible for teaching). The committee of department heads meets quarterly with the president to exchange information.

Hafen wanted to merge some departments into a less unwieldy

number of schools led by professional deans. More contentiously, he sought to reform the *Schulleitung*, eliminating the rector's position and introducing five vice-presidents, whose arrival might have threatened the clout of senior academics.

University professors are notoriously conservative and jealous of their local powers — especially at elite institutions such as the ETH. There might therefore be a tendency to dismiss the brouhaha as academic provincialism. But this would be wrong for two reasons.

First, the ETH professors have in the recent past already cooperated with changes implemented by the president's office. That was a major reason for their reluctance this time: they are still in the process of enacting the last round of reforms, which made departments responsible for their own finances and put in place a new teaching system. They were clearly unconvinced that the time was ripe for reform of these reforms.

And therein lies the second reason. Hafen failed to convince the professors that his proposals made sense, and he declined to engage in the dialogue that might have won them over. Perhaps too confident of the power conferred on him on paper, he failed to talk and, fatally, he failed to listen. He pushed too fast initially and, when an impasse arose, he moved swiftly into reverse, withdrawing his whole reform package in its entirety on 23 October, thereby losing further respect.

The ETH will doubtless survive this embarrassing setback. But Hafen's departure leaves questions about whether his proposals were really being driven by the ETH supervisory council, which hired him but failed to back him when the chips were down. The council must now start afresh, by appointing a president who will inspire the confidence of the university staff. ■

**"Hafen wanted to introduce a more corporate management model at the ETH."**

## Correction or retraction?

Errors reported in this issue by authors of a *Nature* paper pose a dilemma about trust.

The practice of science — and the publication of science in particular — is often lauded for its capacity for self-correction, and, to a large extent, deservedly so. During the peer-review process, basic mistakes and errors of judgement are frequently identified, minimizing the number that make it through into often much-improved final publications. Erroneous results that do slip through the peer-review net may be promptly identified; if sufficiently serious, they are corrected or even withdrawn.

The reality of science publication does not always accord with such

idealistic expectations, however, and the correction published this week (on page 235) is a case in point.

When an important error has been made in a published piece of work, yet the central claim or result still stands, the publication of a Corrigendum is the most sensible way forward; others are thereby alerted to any inaccuracies in the paper, which may have an impact on their own research. If, on the other hand, the errors that have been made undermine the principal message of the paper, then a retraction is in order — the paper may still contain valid scientific information, but the original publication has now lost its *raison d'être*.

There is a grey area in between, exemplified by the events — past and present — that have now culminated in the aforementioned Corrigendum. The original paper (*Nature* 366, 143–146; 1993) is viewed by many as a landmark in its field: an experimental 'first', in which compositional analysis at atomic resolution had been achieved

with an electron microscope. But the paper did not have an easy time with referees, with one reviewer in particular maintaining that there were “disquieting questions” over both the provenance of key data and inconsistencies in the manner in which they had been subsequently reprocessed (in response to concerns raised earlier during the review process) in order to better substantiate the central claim. The authors, however, had provided *Nature* with a robust defence of their work in response to these remaining criticisms — firm assurances that at the time we accepted at face value. Combined with a positive endorsement of the work that was offered by a second referee, we felt it appropriate to proceed with publication of the paper.

Seen with the benefit of hindsight, we made an error of judgement in taking those assurances on trust — perhaps influenced by our awareness of intense competition in the field at the time. For it has belatedly transpired that many of the more critical referee’s “disquieting questions” did indeed have a sound technical basis, as key data were misrepresented by the authors, both during the review process and in the final published version of the paper. This has now been fully acknowledged by the authors, who say that they are mystified as to why they offered the assurances they did when originally challenged on these points.

So what does this mean for the paper? It could be argued, as we have done during extensive deliberations, that confidence in the validity of the work has been severely compromised as a consequence of these errors, and that the paper should be formally retracted. But we have concluded for several reasons that the authors’ Corrigendum should

be accepted. Thirteen years have elapsed since publication, and the authors no longer have available the source data to reanalyse and resubmit to peer review — and so are not in a position to mount a thorough defence of their published results against the remaining criticisms. Furthermore, an investigation commissioned by Oak Ridge National Laboratory in Tennessee has robustly cleared the authors of any intent to deceive; we have received assurances that the original data, if consistently analysed as intended, would still have supported the central thesis of the paper. And most importantly, the authors have both acknowledged and proposed corrections for their earlier mistakes.

In the end, it comes down to an issue that is at the very heart of the practice and communication of science: the question of trust. After all, if researchers and editors cannot safely assume, even as a starting point, that scientific results are essentially true as reported, then the advancement of science is in serious trouble.

Without doubt, there has been in this case a severe breach of the trust on which the publication of science is based. But the reasons underlying it, and the hypothetical outcome for the work had these concerns been tackled more robustly when first raised, can now only be speculated about. Other researchers will have their own take on the situation (see page 129).

There is some consolation in the fact that the experimental capability first reported in the flawed *Nature* paper was soon exceeded, as reported by these authors and others, in a range of different contexts. Thus we can at least be relieved that the progress of science was not impeded by this particular episode. ■

## Smart but lightweight

An imaginative innovation policy in Britain continues to be under-resourced.

It is the intention of every government on Earth to inspire increased research, development and innovation in the private sector. How this should actually be done remains something of a mystery, however. Last week, the British government took a stab at the problem, announcing an administrative change that it hopes will help it meet its ambitious stated goal of expanding business expenditure on research and development from 1.2% of the economy to 1.7% by 2014.

Innovation policy in Britain traditionally falls under the remit of the Department of Trade and Industry (DTI), which has long housed a pot-pourri of small initiatives and programmes aimed at fostering industrial innovation. Two years ago, this mixture was placed under the guidance of the Technology Strategy Board, an advisory committee chaired by Graham Spittle of IBM.

Early next year, the Technology Strategy Board will effectively be spun off from the DTI and reconstituted as an autonomous entity. It will hire a chief executive and a small staff, and will operate at arm’s length from the government, managed by a board drawing members from industry and finance. The group will be constituted much like one of the research councils that support British scientific research, but will have a different mission — fostering innovation in business.

The change will give the group more latitude for effective action, and pulling it out of the DTI will have at least two other significant advantages. It will help the committee to address innovation, not just in manufacturing industry (the DTI’s traditional remit) but also in the service sector — ranging from publishing to banking — which now constitutes four-fifths of Britain’s economy. And the free-standing committee will be better placed to work with all departments of government, and address the area where the state can arguably make the greatest difference of all, by supporting innovative suppliers through the £150 billion (US\$290 billion) or so that it spends each year on goods and services.

However, the resources under the direct control of the new body will remain, in the first instance, rather paltry. Around £170 million worth of grants and other programmes is, for all the talk about intelligent leverage, unlikely to spur much of anything across an economy the size of Britain’s.

The Confederation of British Industry — which has, of course, an interest in the matter — has advocated the spin-off of the Technology Strategy Board, but suggested that it needs four times as much money to have an impact. The question of additional resources will be addressed by the Treasury in next year’s Comprehensive Spending Review. Its outcome will tell us how much faith the government has in this particular innovation. ■

**“The Technology Strategy Board will be constituted much like a research council, but will have a different mission — fostering innovation in business.”**

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THIS STORY HAS BEEN FORMATTED FOR EASY PRINTING

## **Oak Ridge researchers admit errors**

**The Boston Globe**

By Eugenie Samuel Reich, Globe Correspondent | November 27, 2006

Thirteen years after the fact, scientists at a top US Department of Energy laboratory have admitted misrepresenting key data in a landmark paper on the use of electron microscopes to analyze materials at the atomic scale.

Publication of the correction earlier this month in the science journal *Nature* was more than a historical footnote. It followed an allegation that scientists in the same lab had manipulated data in a new paper submitted to a sister journal. The allegation, made by a reviewer for *Nature Physics*, was confidential.

Word of it circulated unofficially among scientists, however, and several have now raised broader concerns about the reliability of the work of the team at Oak Ridge National Laboratory in Tennessee, which is led by Stephen Pennycook and gets about \$2 million a year from taxpayers.

Pennycook said the data problems were mistakes that didn't undermine the papers' conclusions. But John Spence, a physics professor at Arizona State University with a joint appointment at the Energy Department's Lawrence Berkeley National Laboratory, said they are "very troubling. . . . This is a field that involves the use of very expensive, highly centralized facilities, and Pennycook's group is the best funded."

In recent years, a number of high-profile instances of scientific fraud -- most famously a Korean team's claim that it cloned human embryonic stem cells -- have made clear the limits of peer review by outside scientists to flag problematic papers before they are published. But the Oak Ridge case highlights the fact that even when peer reviewers suspect that authors are manipulating or fabricating data, there is no certainty other scientists will be alerted to their concerns.

In some cases, reviewers may be hesitant to get involved in a messy situation and simply recommend rejection of the paper. If they do inform editors, the editors are barred from speaking publicly, though they can notify the authors' institution.

This can leave authors free to revise the paper and shop it around to other journals with a less rigorous review process.

Karl Ziemelis, *Nature*'s physical sciences editor, said the journal is unable to publicly discuss submitted manuscripts, even ones with serious problems, because they are confidential. "In general, there is nothing sinister about this -- one of the key purposes of peer review is to identify honest mistakes, which may subsequently be corrected," he said. "But, of course, peer review confidentiality could be exploited."

This possibility was envisioned by the reviewer for *Nature Physics* in April. "I find that there is direct, incontrovertible evidence for systemic data manipulation and scientific misconduct in this manuscript," the reviewer wrote about a paper whose lead author was Maria Varela, a staff scientist in Pennycook's group. The comments were provided to the *Globe* on the condition the reviewer not be identified.

One example the reviewer cited was a figure that showed the number of electrons detected by the Oak Ridge electron microscope as it scanned across a three-layer sandwich, with one material in the middle flanked on each side by a second material. The data points for the outside layers were exact mirror images, something that would be implausible. In addition, the data points for the middle layer were an inverted version of data for a different sample of the material.

The reviewer went on to raise the concern that the comments might "effectively 'aid and abet' improper behavior," enabling the authors to quietly correct or remove the evidence of misconduct from their manuscript and resubmit it.

The reviewer also pointed out that similar problems were evident in other papers published by Varela and urged the editors to notify the authors' institutions.

James Roberto, deputy director for science and technology at Oak Ridge, said he convened a panel of three outside scientists to examine allegations received from Nature in May, and they cleared Pennycook's group of misconduct in July. "This is not a case of research misconduct," he said, only a case of errors in the group's work.

Pennycook and Varela acknowledged in an interview that in the "sandwich" figure cited by the reviewer, measurements had not been taken for one of the outside layers and data from the opposite layer were used instead for illustrative purposes. "I think this was in a sense schematic," said Pennycook. The data shown for the middle layer were measured on a different sample and switched in by mistake, they said. Varela said other results in the manuscript were taken from a 2003 paper she published and mislabeled.

Several scientists questioned the use of mirrored data, because the figure was labeled as actual measured data. "That is an inventive step the rest of us wouldn't have made. The point in science is to be accurate and not about presentation," said Neil Mathur, a materials scientist at Cambridge University in England.

Misrepresented data also were at issue in the 1993 paper.

"Key data were misrepresented by the authors, both during the review process and in the final published version of the paper," Nature said in an editorial that accompanied the correction published Nov. 9. "Without doubt, there has been . . . a severe breach of the trust on which the publication of science is based." Pennycook was a co-author of that paper, but not Varela.

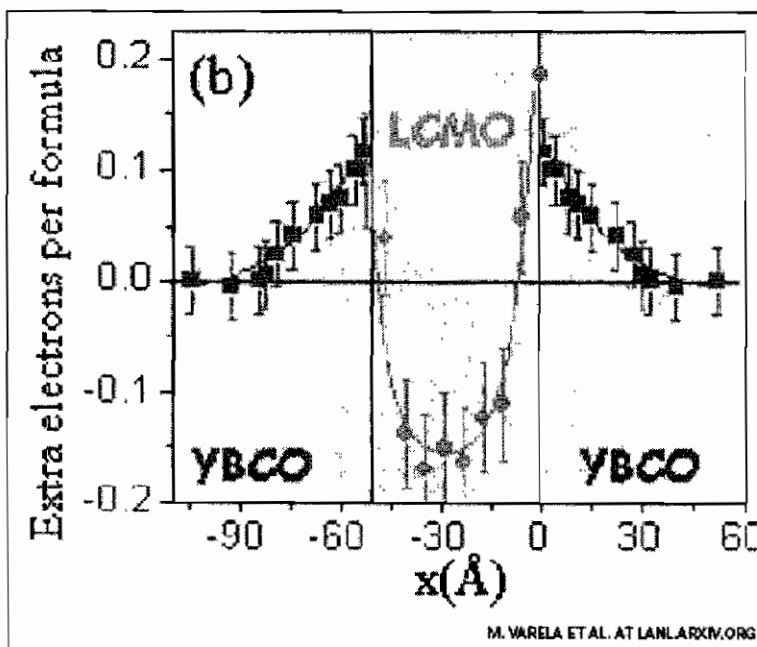
Since the correction was published, scientists have questioned four additional papers by Pennycook and Varela, noting that figures supposedly showing the same results have data points in different places. Pennycook told the Globe he will correct a figure in one of the papers but said the other discrepancies resulted from reanalysis of the data.

"All the mistakes uncovered in our publications are editorial in nature, regrettable, and without impact on the scientific conclusions," he wrote in an e-mail. ■

## Extra electrons per formula

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This figure, posted on a website scientists use to share unpublished manuscripts, is similar to one in the paper submitted to Nature Physics by Oak Ridge National Laboratory researchers. It shows electron microscope measurements of a three-layer "sandwich" of materials, but the data points for the layer on the left are not actual measurements; they are a mirror image of the data points on the right. In addition, the data points for the middle layer are an inverted version of data for a different sample of the material. The researchers have posted a revised version of this figure.

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## Scientists acknowledge 'inconsistencies' in data published 13 years ago

**BYLINE:** Frank Munger, The Knoxville News-Sentinel, Tenn.

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Dec. 1--OAK RIDGE -- At the peak of a brilliant scientific career, Steve Pennycook is having to defend his reputation.

"It's difficult," Pennycook, 53, said in a telephone interview this week from Boston, where he was attending a conference of the Materials Research Society.

He was the talk of the town, at least in scientific circles, and for once in his life, that wasn't a good thing. Just about everybody at the conference knew of the emerging controversy regarding the work of Pennycook and colleagues at Oak Ridge National Laboratory.

In the November issue of *Nature*, a British journal that is among the world's most prestigious places in which to publish scientific findings, Pennycook and two co-authors wrote a corrigendum -- a correction of errors -- for an important paper published 13 years earlier.

Pennycook, a native of Kent, England, is a corporate fellow at ORNL and was chosen the lab's "scientist of the year" in 2005. He's considered one of the world's leading microscopists, and his research team established a record for image resolution in an experiment a couple of years ago.

The 1993 paper, "Atomic resolution chemical analysis using a scanning transmission electron microscope," has been termed a landmark piece of science. It documented the ability to look at individual atoms to analyze the composition of a material.

After the work was challenged earlier this year in a confidential report to *Nature*, the Oak Ridge team acknowledged there were "inconsistencies" in the way key data were presented. Basically, they admitted that they didn't do things exactly like they said they did in the paper and as they had assured the editors of *Nature* at the time.

The scientists said the errors did not affect the paper's scientific conclusions.

An investigation team convened by ORNL cleared the researchers of misconduct on that and another paper that aroused suspicions and allegations this year, said Jim Roberto, ORNL's deputy director for science and technology.



"We take allegations of this type very serious," Roberto said, noting that a three-person team from academic institutions conducted the review that took most of the summer to complete.

"The overall finding of the report was there was no evidence of research misconduct. There were some errors in the papers but they were not intentional," ORNL's research administrator said.

Rival scientists, however, have suggested that there's more going on than a minor bout of sloppiness, and one scientist, John Silcox of Cornell University told Nature, "It's obvious that some games are being played. I don't trust their work."

Nature even wrote an editorial to discuss the issue and explain why it decided not to retract the 1993 paper in its entirety.

"Without doubt, there has been in this case a severe breach of trust on which the publication of science is based," the editorial states.

"After all," the editors noted, "if researchers and editors cannot safely assume, even as a starting point, that scientific results are essentially true as reported, then the advancement of science is in serious trouble."

Nature chose not to retract the paper because the essence of the science was still intact.

In their correction, the ORNL authors, including Nigel Browning (now at the University of California at Davis) and Matt Chisholm, admitted to "inconsistencies" in the way key data were presented.

"In particular, the electron energy-loss spectroscopy data central to the work were not subject to the background subtraction processes as described in the paper, despite the assurances to the contrary that we offered at the time to both the referees and the Nature editors," they wrote.

Other issues were raised about the handling of scientific results in another paper that was submitted to and rejected by Nature Physics, a sister publication, earlier this year. Pennycook was a co-author on that paper, which was headed by Maria Valera of ORNL.

Pennycook insisted that there was no attempt to gain a scientific advantage in the highly competitive field. He said he realized his entire body of work would now come under greater scrutiny as a result of the problems.

"It's very embarrassing, and it does undermine confidence in what we do," Pennycook said. "That's the extent of it I think most people in the community, if all their papers were put under the microscope, there'd be some embarrassments in there."

He said he did not think his research funding, which comes from the U.S. Department of Energy, would be affected.

Roberto said he wasn't sure what the impact would be on ORNL, which has been on a positive roll in recent years and lays claim to being DOE's top scientific laboratory. The lab staff publishes about 1,500 research papers annually, he said.

"We don't see a sinister, dark side," he said. "We should have been more careful I believe we did a robust review. I also believe we learned some lessons here internally in terms of the risk that staff encounter if they make mistakes."

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